Contents to Volumes 427–428

Preface xv

Conference organisation xvi

1. Surface dynamics

Determination of the lateral potential energy surface of single adsorbed atoms and molecules on single crystal surfaces using helium atom scattering
A.P. Graham and J.P. Toennies 1

Accurate and efficient determination of chemisorption energies using pseudopotentials
E.J. Walter and A.M. Rappe 11

The role of vibrational entropy in surface diffusion: adatoms and vacancies on Ag(100), Cu(100), and Ni(100)
U. Kürpick and T.S. Rahman 15

Vibrational spectroscopy of water molecules on Pt(111) at submonolayer coverages
A.L. Glebov, A.P. Graham and A. Menzel 22

Angular distributions of NO in laser-induced desorption from Pt(111)
M. Wilde, K. Fukutani, Y. Murata, M. Kampling, K. Al-Shamery and H.-J. Freund 27

Optical decoherence and quantum beats in Cs/Cu(111)
S. Ogawa, H. Nagano and H. Petek 34

Lateral thermal expansion of Cu(110) surface studied with helium atom scattering
T. Miyake, I. Oodake and H. Petek 39

2. Phonon dispersion

High-resolution analysis of semiconductor surface phonons by Raman spectroscopy
N. Esser, K. Hinrichs, J.R. Power and W. Richter 44

Stability and lattice vibrations of the clean diamond (111) surface
M. Saito, Y. Miyamoto and A. Oshiyama 53

Density-functional calculation of phonons in adsorbate-covered semiconductor surfaces
J. Fritsch, M. Arnold, C. Eckl, R. Honke, P. Pavone and U. Schröder 58

Collective vibrational modes of the high-density (1 × 1)-O phase on Ru(001)
T. Moritz, D. Menzel and W. Widdra 64

Determination of six types of vibrational mode for bridge CO on Pd(110)
H. Kato, J. Yoshinobu and M. Kawai 69

3. New surface phases and thin layers

Structure and chemistry of Pd(100)-p(2 × 2)-p4g–Al surface alloy
K. Kishi, A. Oka, N. Takagi, M. Nishijima and T. Aruga 74

HREELS, IR and SFG investigation of undoped and doped adsorbed fullerenes
C. Silien, Y. Caudano, J.-L. Longueville, S. Bouzidi, F. Wiame, A. Peremans and P.A. Thiry 79

Bonding nature of C_{60} adsorbed on Si(111)7 × 7 and Si(100)2 × 1 surfaces studied by HREELS and PES
S. Suto, K. Sakamoto, D. Kondo, T. Wakita, A. Kimura and A. Kakizaki 85

Combined EELS/1STM study of the adsorption of nitric oxide and the formation of GaO_xN_y on CoGa(001)
G. Schmitz, M. Eumann, D. Stapel and R. Franchy 91

Vibrational spectra of the monolayer films of hexagonal boron nitride and graphite on faceted Ni(755)
E. Rokuta, Y. Hasegawa, A. Itoh, K. Yamashita, T. Tanaka, S. Otani and C. Oshima 97

An infrared spectroscopic study of water thin films on NaCl(100)
M. Foster and G.E. Ewing 102

Infrared studies of mixed Langmuir–Blodgett monolayers of octadecyldimethylamine oxide and dioctadecyldimethylammonium chloride with arachidic acid and poly(acrylic acid)
D.A. Myrzakozha, T. Hasegawa, J. Nishijo, T. Imae and Y. Ozaki 107

Surface-enhanced Raman scattering study of organic thin films of 2-octadecyl-7,7,8,8-tetracyanoquinodimethane and its charge transfer films doped with 3,3′,5,5′-tetramethylbenzidine
Y.M. Jung, H. Sato, T. Ikeda, H. Tashiro and Y. Ozaki 111

4. Optical methods and instrumentation

Surface enhanced Raman scattering as a probe of adsorbate–substrate charge-transfer excitations
P. Kambhampati and A. Campion 115

Enhanced-Raman scattering from organic thin films mediated by half-leaky guided modes
S. Hayashi, T. Kitagawa, Y. Sekiguchi and T. Kume 126

Enhancement of optical second harmonic response mediated by half-leaky guided modes
H. Sano, G. Mizutani, S. Ushioda, T. Kitagawa, T. Kume and S. Hayashi 131

Thickness dependence of infra-red absorption enhancement for methanol on evaporated silver films
Y. Suzuki, H. Seki, T. Inamura, T. Tanabe, T. Wadayama and A. Hatta 136

Imaging and spectroscopic analysis of single microdroplets containing *p*-cresol using the near-infrared laser tweezers/Raman microprobe system
K. Ajito and M. Morita 141

Excitation energy profile of the SH intensity from a glass–Au interface
H. Tanaka, H. Wakimoto, T. Miyazaki, G. Mizutani and S. Ushioda 147

Effect of shear horizontal leaky surface acoustic wave on selectivity for ethanol decomposition of a copper thin-film catalyst deposited on a positively polarized ferroelectric $LiTaO_3$ single crystal
H. Nishiyama, N. Saito, T. Yashima, K. Sato and Y. Inoue 152

5. Electrochemistry

Extending surface Raman spectroscopic studies to transition metals for practical applications. II. Hydrogen adsorption at platinum electrodes
B. Ren, X. Xu, X.Q. Li, W.B. Cai and Z.Q. Tian 157

Extending surface Raman spectroscopic studies to transition metals for practical applications. III. Effects of surface roughening procedure on surface-enhanced Raman spectroscopy from nickel and platinum electrodes
Q.J. Huang, X.Q. Li, J.L. Yao, B. Ren, W.B. Cai, J.S. Gao, B.W. Mao and Z.Q. Tian 162

Adsorption of urea on Au(100) and Au(111) electrode surfaces studied by in-situ Fourier-transform infra-red spectroscopy
M. Nakamura, M.-B. Song and M. Ito 167

Coadsorption of ammonia and electrolyte anions on a Pt(111) electrode
Y. Shingaya, H. Kubo and M. Ito 173

In-situ ATR-IR study of water on gold electrode surface
M. Futamata 179

In situ infrared monitoring of hydrogen adsorption/desorption at a germanium electrode
F. Maroun, F. Ozanam and J.-N. Chazalviel 184

Time-resolved surface-enhanced infra-red study of molecular adsorption at the electrochemical interface
H. Noda, K. Ataka, L.-J. Wan and M. Osawa 190

Electrochemical reaction of $Fe(CN)_6^{3-,4-}$ on gold electrodes analyzed by surface plasmon resonance
Y. Iwasaki, T. Horiuchi, M. Morita and O. Niwa 195

6. Semiconductor surfaces

In-situ IR observation of etching and oxidation processes of Si surfaces
M. Niwano 199

Hydrogen-terminated Si(111) and Si(100) by wet chemical treatment: linear and non-linear infrared spectroscopy
C. Mazzara, J. Jupille, W.-Q. Zheng, M. Tanguy, A. Tadjeddine and P. Dumas 208

Formation and decomposition of a Si hydride layer during vacuum ultraviolet-excited Si homoepitaxy from disilane
H. Akazawa 214

Dependence of interface states for ultra-thin SiO_2/Si interfaces on the oxide atomic density determined from FTIR measurements
A. Asano, T. Kubota, Y. Nishioka and H. Kobayashi 219

Metal–semiconductor transition observed by HREELS on the surface of $Si_{1-x}Ge_x$/Si(001) grown by CTL-CVD at 620 K
T. Angot and P. Louis 224

Observation of Ge surface segregation during Si-MBE on Ge/Si(001) probed by Si–H/Ge–H surface vibrations
Y. Kobayashi, K. Sumitomo and T. Ogino 229

Enhancement of adsorbate vibrations due to interaction with microcavity mode in porous silicon superlattice
G. Mattei, E.V. Alieva, J.E. Petrov and V.A. Yakovlev 235

Photoconductivity of the Si(111)-7×7 and $\sqrt{3} \times \sqrt{3}$-Ag surfaces
C.-S. Jiang and S. Hasegawa 239

Infrared spectroscopy of C–D vibrational modes on diamond (100) surfaces
L. Ley, B.F. Mantel, K. Matura, M. Stammler, K. Janischowsky and J. Ristein 245

Structural, vibrational and electronic properties of faceted GaN(000$\bar{1}$) surfaces
S. Sloboshanin, F.S. Tautz, V.M. Polyakov, U. Starke, A.S. Usikov, B.Ja. Ber and J.A. Schaefer 250

Combined HREELS/LEED study on the oxidation of GaN surfaces
T. Tsuruoka, M. Kawasaki, S. Ushioda, R. Franchy, Y. Naoi, T. Sugahara, S. Sakai and Y. Shintani 257

7. Chemical reactions

The formation of carbonate on Ag(110) studied by high-resolution EELS
L. Constant, B. Krenzer, W. Stenzel, H. Conrad and A.M. Bradshaw 262

Ethylene hydrogenation on a Ni(100) surface
C. Egawa, S. Oki, M. Kaneko, N. Minami and I. Suzuki 268

Site switching in steady state carbon monoxide oxidation on platinum(113)
G. Cao, G. Moula, Y. Ohno and T. Matsushima 272

A new reaction channel in H(g) + D(a)/Pd(100): absorption versus abstraction
H. Okuyama, T. Nakagawa, W. Siga, N. Takagi, M. Nishijima and T. Aruga 277

Infrared studies of sub-monolayer methylamine and trimethylamine adsorption on Ni(111)
T.S. Nunney, J.J. Birtill and R. Raval 282

Oxide-supported Rh particle structure probed with carbon monoxide
M. Frank, R. Kühnemuth, M. Bäumer and H.-J. Freund 288

SHG observation of *rutile* $TiO_2(110)/H_2O$ interface under UV light illumination
E. Kobayashi, K. Matsuda, G. Mizutani and S. Ushioda 294

Chemical reactions of ammonia with polar and non-polar nitride semiconductor surfaces
J. Fritsch, O.F. Sankey, K.E. Schmidt and J.B. Page 298

In situ FT-IR and photoluminescence study of porous silicon during exposure to F_2, H_2O, and D_2O
T. Arigane, K. Yoshida, T. Wadayama and A. Hatta 304

8. Vibrational dynamics

Lateral interactions in (NO + O) coadsorbate layers on Ru(001): fundamental and overtone modes
P. Jakob 309

Surface Raman scattering study on the hydrogenated semiconductor surfaces: vibrational dephasing dynamics
C.-S. Tsai, C. Chen, C.-E. Lin, J.-C. Lin and J.-K. Wang 318

Influence of pulse duration on time-resolved sum-frequency generation on surface vibrations
T. Mii and H. Ueba 324

Time-resolved SFG study of the vibrational excitation of adsorbed CO on Ni(111) and NiO(111) surfaces under the irradiation of UV and visible photons
A. Bandara, J. Kubota, K. Onda, A. Wada, S.S. Kano, K. Domen and C. Hirose 331

Screening of SFG signals from bridged CO on Ni(111) by the coexistence of linear CO
S. Katano, A. Bandara, J. Kubota, K. Onda, A. Wada, K. Domen and C. Hirose 337

Classical and quantum mechanical studies of the CO vibrations in CO/Cu(100)
S.C. Park, W.K. Park and J.M. Bowman 343

9. Dynamics in chemical processes

SFG study of unstable surface species by picosecond pump–probe method
K. Domen, A. Bandara, J. Kubota, K. Onda, A. Wada, S.S. Kano and C. Hirose 349

Rotational polarization and filtering of hydrogen molecules by metal surfaces – isotope effects
W.A. Diño, H. Kasai and A. Okiji 358

CO_2 desorption induced by photo-excitation, photo-reaction, and hot-atom collision on a stepped platinum (113) surface
T. Yamanaka, Y. Shimizu, E. Kitayama and T. Matsushima 364

The influence of coadsorbed sodium atoms on the chemisorption of benzoic acid on Si(100)-2 × 1
T. Bitzer and N.V. Richardson 369

10. Adsorption

Infrared reflection absorption spectroscopic study on the adsorption structures of ethylene on Ag(110) and atomic oxygen pre-covered Ag(110) surfaces
M. Akita, N. Osaka, S. Hiramoto and K. Itoh 374

Infrared reflection–absorption spectroscopic study on the adsorption structures of acrylonitrile on Ag(111) and Ag(110) surfaces
N. Osaka, M. Akita, S. Hiramoto and K. Itoh 381

Physisorption of a long-chain *n*-alkane on Ag(111) surface: an infra-red reflection absorption spectroscopic study
M. Yamamoto, Y. Sakurai, Y. Hosoi, H. Ishii, E. Ito, K. Kajikawa, Y. Ouchi and K. Seki 388

Adsorption state of diethyldisulfide on Au(111) studied with a combined system of HREELS and STM
T. Hayashi, A. Fricke, K. Katsura, C. Kodama and H. Nozoye 393

Adsorption properties of ethene on $Pt_3Cu(111)$
T. Pelster, C. Becker, M. Tanemura, J. Breitbach and K. Wandelt 398

CO adsorption on $Cu_3Pt(111)$ and $CuPt_3(111)$: a comparative HREELS study
C. Becker, T. Pelster, M. Tanemura, J. Breitbach and K. Wandelt 403

CO-induced destruction of Cu(100)-(2 × 1)Li studied by HREELS
T. Sasaki, R. Tero, T. Sueyoshi and Y. Iwasawa 408

Carbon monoxide adsorption on ultra-thin Fe film deposited on Cu(100)
T. Tanabe, Y. Suzuki, T. Wadayama and A. Hatta 414

Molecular orbital study of the interactions of CO molecules adsorbed on a W(111) surface
G.H. Ryu, S.C. Park and S.-B. Lee 419

Polarization infrared spectroscopic study of the influence of external lateral electric fields up to 8×10^5 V m^{-1} on the CO_2–NaCl(100) adsorbate
J. Heidberg, A. Rugullies, I. Stahl and M. Thomas 426

Davydov and site symmetry splitting in polarized infrared spectra of ordered monolayers. A quantitative theoretical analysis of vibrational frequencies and integrated absorptions for CO_2 on NaCl(100)
J. Heidberg, M. Hustedt, E. Kampshoff and V.M. Rozenbaum 431

The physisorption of CO_2 and the stepwise chemisorption of SO_2 on the CsF(100) single crystal surface
J. Heidberg and H. Henseler 439

Complementary vibrational and reflectance anisotropy spectroscopic determination of molecular azimuthal orientation
C.C. Perry, B.G. Frederick, J.R. Power, R.J. Cole, S. Haq, Q. Chen, N.V. Richardson and P. Weightman 446

Author index 452

Subject index 457

Materials index 467